# BEC, BCS AND BCS-BOSE CROSSOVER THEORIES IN SUPERCONDUCTORS AND SUPERFLUIDS

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#### 1. INTRODUCTION

Though commonly unrecognized, a superconducting BCS condensate consists of equal numbers of two-electron (2e) and two-hole (2h) Cooper pairs (CPs). A complete boson-fermion (statistical) model (CBFM), however, is able to depart from this perfect 2e-/2h-CP symmetry and yields [1] robustly higher  $T_c$ 's without abandoning electron-phonon dynamics mimicked by the BCS/Cooper model interaction  $V_{\mathbf{k},\mathbf{k}'}$  which is a nonzero negative constant -V, if and only if single-particle energies  $\epsilon_k$ ,  $\epsilon_{k'}$  are within an interval  $[\max\{0, \mu - \hbar\omega_D\}, \mu + \hbar\omega_D]$  where  $\mu$  is the electron chemical potential and  $\omega_D$  is the Debye frequency. The CBFM is "complete" only in the sense that 2h-CPs are not ignored, and reduces to all the known statistical theories of superconductors (SCs), including the BCS-Bose "crossover" picture but goes considerably beyond it.

Boson-fermion (BF) models of SCs as a Bose-Einstein condensation (BEC) go back to the mid-1950's [2-5], pre-dating even the BCS-Bogoliubov theory [6-8]. Although BCS theory only contemplates the presence of "Cooper correlations" of single-particle states, BF models [2-5, 9-17] posit the existence of actual bosonic CPs. Indeed, CPs appear to be universally accepted as the single most important ingredient of SCs, whether conventional or "exotic" and whether of low- or high-transition-temperatures  $T_c$ . In spite of their centrality, however, they are poorly understood. The fundamental drawback of early [2-5] BF models, which took 2e bosons as analogous to diatomic molecules in a classical atom-molecule gas mixture, is the notorious absence of an electron energy gap  $\Delta(T)$ . "Gapless" models cannot describe the superconducting state at all, although they are useful [16,17] in locating transition

temperatures if approached from above, i.e.,  $T > T_c$ . Even so, we are not aware of any calculations with the early BF models attempting to reproduce any empirical  $T_c$  values. The gap first began to appear in later BF models [9-14]. With two [12, 13] exceptions, however, all BF models neglect the effect of *hole* CPs accounted for on an equal footing with electron CPs, except the CBFM which consists of *both* bosonic CP species coexisting with unpaired electrons, in a *ternary* gas mixture. Unfortunately, no experiment has yet been performed, to our knowledge, that distinguishes between electron and hole CPs.

The "ordinary" CP problem [18] for two distinct interfermion interactions (the  $\delta$ -well [19, 20] or the Cooper/BCS model [6, 18] interactions) neglects the effect of 2h CPs treated on an equal footing with 2e [or, in general, two-particle (2p)] CPs. On the other hand, Green's functions [21] can naturally deal with hole propagation and thus treat both 2e- and 2h-CPs [22, 23]. In addition to the generalized CP problem, a crucial result [12, 13] is that the BCS condensate consists of equal numbers of 2p and 2h CPs. This was already evident, though widely ignored, from the perfect symmetry about  $\epsilon = \mu$  of the well-known Bogoliubov [24]  $v^2(\epsilon)$  and  $u^2(\epsilon)$  coefficients, where  $\epsilon$  is the electron energy.

Here we show: a) how the crossover picture  $T_c$ s, defined self-consistently by both the gap and fermion-number equations, requires unphysically large couplings (at least for the Cooper/BCS model interaction in SCs) to differ significantly from the  $T_c$  from ordinary BCS theory defined without the number equation since here the chemical potential is assumed equal to the Fermi energy; how although ignoring either 2h- or 2e-CPs in the CBFM b) one obtains the precise BCS gap equation for all temperatures T, but c) only half the T=0 BCS condensation energy emerges. The gap equation gives  $\Delta(T)$  as a function of coupling, from which  $T_c$  is found as the solution of  $\Delta(T_c)=0$ . The condensation energy is simply related to the ground-state energy of the many-fermion system, which in the case of BCS is a rigorous upper bound to the exact many-body value for the given Hamiltonian. Results (b) and (c) are also expected to hold for neutral-fermion superfluids (SFs)—such as liquid <sup>3</sup>He [25, 26], neutron matter and trapped ultra-cold fermion atomic gases [27-38]—where the pair-forming two-fermion interaction of course differs from the Cooper/BCS one for SCs.

## 2. THE COMPLETE BOSON-FERMION MODEL

The CBFM [12, 13] is described in d dimensions by the Hamiltonian  $H = H_0 + H_{int}$ . The unperturbed Hamiltonian  $H_0$  corresponds to a non-Fermi-liquid "normal" state, being an ideal (i.e., noninteracting) ternary gas mixture of unpaired fermions and both types of CPs namely, 2e and 2h. It is

$$H_0 = \sum_{\mathbf{k_1}, \mathbf{s_1}} \epsilon_{\mathbf{k_1}} a_{\mathbf{k_1}, \mathbf{s_1}}^+ a_{\mathbf{k_1}, \mathbf{s_1}} + \sum_{\mathbf{K}} E_+(K) b_{\mathbf{K}}^+ b_{\mathbf{K}} - \sum_{\mathbf{K}} E_-(K) c_{\mathbf{K}}^+ c_{\mathbf{K}}$$

where as before  $\mathbf{K} \equiv \mathbf{k_1} + \mathbf{k_2}$  is the CP center-of-mass momentum (CMM) wavevector while  $\epsilon_{\mathbf{k_1}} \equiv \hbar^2 k_1^2/2m$  are the single-electron, and  $E_{\pm}(K)$  the 2e-/2h-CP phenomenological, energies. Here  $a_{\mathbf{k_1},\mathbf{s_1}}^+$  ( $a_{\mathbf{k_1},\mathbf{s_1}}$ ) are creation (annihilation) operators for fermions

and similarly  $b_{\mathbf{K}}^{+}$  ( $b_{\mathbf{K}}$ ) and  $c_{\mathbf{K}}^{+}$  ( $c_{\mathbf{K}}$ ) for 2e- and 2h-CP bosons, respectively. Two-hole CPs are considered distinct and kinematically independent from 2e-CPs.

The interaction Hamiltonian  $H_{int}$  (simplified by dropping all  $\mathbf{K} \neq \mathbf{0}$  terms, as is done in BCS theory in the *full* Hamiltonian but kept in the CBFM in  $H_0$ ) consists of four distinct BF interaction vertices each with two-fermion/one-boson creation and/or annihilation operators. The vertices depict how unpaired electrons (subindex +) [or holes (subindex -)] combine to form the 2e- (and 2h-) CPs assumed in the d-dimensional system of size L, namely

$$H_{int} = L^{-d/2} \sum_{\mathbf{k}} f_{+}(k) \{ a_{\mathbf{k},\uparrow}^{+} a_{-\mathbf{k},\downarrow}^{+} b_{\mathbf{0}} + a_{-\mathbf{k},\downarrow} a_{\mathbf{k},\uparrow} b_{\mathbf{0}}^{+} \}$$

$$+ L^{-d/2} \sum_{\mathbf{k}} f_{-}(k) \{ a_{\mathbf{k},\uparrow}^{+} a_{-\mathbf{k},\downarrow}^{+} c_{\mathbf{0}}^{+} + a_{-\mathbf{k},\downarrow} a_{\mathbf{k},\uparrow} c_{\mathbf{0}} \}$$
(1)

where  $\mathbf{k} \equiv \frac{1}{2}(\mathbf{k_1} - \mathbf{k_2})$  is the relative wavevector of a CP. The interaction vertex form factors  $f_{\pm}(k)$  in (1) are essentially the Fourier transforms of the 2e- and 2h-CP intrinsic wavefunctions, respectively, in the relative coordinate of the two fermions. In Refs. [12, 13] they are taken as

$$f_{\pm}(\epsilon) = \begin{cases} f & \text{if } \frac{1}{2} [E_{\pm}(0) - \delta \varepsilon] < \epsilon < \frac{1}{2} [E_{\pm}(0) + \delta \varepsilon] \\ 0 & \text{otherwise.} \end{cases}$$
 (2)

One then introduces the quantities  $E_f$  and  $\delta \varepsilon$  as new phenomenological dynamical energy parameters (in addition to the positive BF vertex coupling parameter f) that replace the previous  $E_{\pm}(0)$  parameters, through the definitions

$$E_f \equiv \frac{1}{4} [E_+(0) + E_-(0)] \quad \text{and} \quad \delta \varepsilon \equiv \frac{1}{2} [E_+(0) - E_-(0)]$$
 (3)

where  $E_{\pm}(0)$  are the (empirically unknown) zero-CMM energies of the 2e- and 2h-CPs, respectively. Alternately, one has the two relations

$$E_{\pm}(0) = 2E_f \pm \delta\varepsilon. \tag{4}$$

The quantity  $E_f$  serves as a convenient energy scale; it is not to be confused with the Fermi energy  $E_F = \frac{1}{2}mv_F^2 \equiv k_BT_F$  where  $T_F$  is the Fermi temperature. The Fermi energy  $E_F$  equals  $\pi\hbar^2 n/m$  in 2D and  $(\hbar^2/2m)(3\pi^2n)^{2/3}$  in 3D, with n the total number-density of charge-carrier electrons, while  $E_f$  is the same with n replaced by, say,  $n_f$ . The quantities  $E_f$  and  $E_F$  coincide only when perfect 2e/2h-CP symmetry holds, i.e. when  $n = n_f$ .

The grand potential  $\Omega$  for the full  $H = H_0 + H_{int}$  is then constructed via

$$\Omega(T, L^d, \mu, N_0, M_0) = -k_B T \ln \left[ \text{Tr} e^{-\beta(H - \mu \hat{N})} \right]$$
(5)

where "Tr" stands for "trace." Following the Bogoliubov recipe [39], one sets  $b_{\mathbf{0}}^+$ ,  $b_{\mathbf{0}}$  equal to  $\sqrt{N_0}$  and  $c_{\mathbf{0}}^+$ ,  $c_{\mathbf{0}}$  equal to  $\sqrt{M_0}$  in (1), where  $N_0$  is the T-dependent number

of zero-CMM 2e-CPs and  $M_0$  the same for 2h-CPs. This allows *exact* diagonalization, through a Bogoliubov transformation, giving [40]

$$\frac{\Omega}{L^d} = \int_0^\infty d\epsilon N(\epsilon) [\epsilon - \mu - E(\epsilon)] - 2k_B T \int_0^\infty d\epsilon N(\epsilon) \ln\{1 + \exp[-\beta E(\epsilon)]\} 
+ [E_+(0) - 2\mu] n_0 + k_B T \int_{0^+}^\infty d\epsilon M(\epsilon) \ln\{1 - \exp[-\beta \{E_+(0) + \epsilon - 2\mu\}]\} 
+ [2\mu - E_-(0)] m_0 + k_B T \int_{0^+}^\infty d\epsilon M(\epsilon) \ln\{1 - \exp[-\beta \{2\mu - E_-(0) + \epsilon\}]\}$$
(6)

where  $N(\epsilon)$  and  $M(\varepsilon)$  are respectively the electronic and bosonic density of states,  $E(\epsilon) = \sqrt{(\epsilon - \mu)^2 + \Delta^2(\epsilon)}$  where  $\Delta(\epsilon) \equiv \sqrt{n_0} f_+(\epsilon) + \sqrt{m_0} f_-(\epsilon)$ , with  $n_0(T) \equiv N_0(T)/L^d$  and  $m_0(T) \equiv M_0(T)/L^d$  being the 2e-CP and 2h-CP number densities, respectively, of BE-condensed bosons. Minimizing (6) with respect to  $N_0$  and  $M_0$ , while simultaneously fixing the total number N of electrons by introducing the electron chemical potential  $\mu$ , namely

$$\frac{\partial\Omega}{\partial N_0} = 0, \qquad \frac{\partial\Omega}{\partial M_0} = 0, \qquad \text{and} \qquad \frac{\partial\Omega}{\partial\mu} = -N$$
 (7)

specifies an equilibrium state of the system with volume  $L^d$  and temperature T. Here N evidently includes both paired and unpaired CP electrons. The diagonalization of the CBFM H is exact, unlike with the BCS H, so that the CBFM goes beyond mean-field theory. Some algebra then leads [40] to the three coupled integral Eqs. (7)-(9) of Ref. [12]. Self-consistent (at worst, numerical) solution of these three coupled equations then yields the three thermodynamic variables of the CBFM

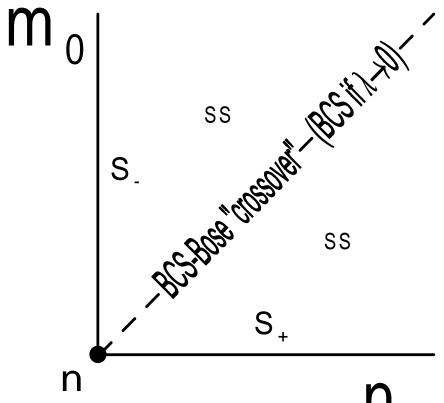
$$n_0(T, n, \mu), \quad m_0(T, n, \mu), \quad \text{and} \quad \mu(T, n).$$
 (8)

Fig.1 displays the three BE condensed phases—labeled s+, s- and ss—along with the normal phase n, that emerge [13] from the CBFM.

Vastly more general, the CBFM contains [1] the key equations of all five distinct statistical theories as special cases; these range from BCS to BEC theories, which are thereby unified by the CBFM. Perfect 2e/2h CP symmetry signifies equal numbers of 2e- and 2h-CPs, more specifically,  $n_B(T) = m_B(T)$  as well as  $n_0(T) = m_0(T)$ . With (4) this implies that  $E_f$  coincides with  $\mu$ , and the CBFM then reduces to the gap and number equations [viz., (11) and (12) below] of the BCS-Bose crossover picture with the Cooper/BCS model interaction—if its parameters V and  $\hbar\omega_D$  are identified with the BF interaction Hamiltonian  $H_{int}$  parameters  $f^2/2\delta\varepsilon$  and  $\delta\varepsilon$ , respectively. The crossover picture for unknowns  $\Delta(T)$  and  $\mu(T)$  is now supplemented by the central relation

$$\Delta(T) = f\sqrt{n_0(T)} = f\sqrt{m_0(T)}. (9)$$

Both  $\Delta(T)$  and  $n_0(T)$  and  $m_0(T)$  are the familiar "half-bell-shaped" order-parameter curves. These are zero above a certain critical temperature  $T_c$ , rising monotonically upon cooling (lowering T) to maximum values  $\Delta(0)$ ,  $n_0(0)$  and  $m_0(0)$  at T=0. The energy gap  $\Delta(T)$  is the order parameter describing the superconducting (or



**Figure 1.** Illustration in the  $n_0$ - $m_0$  plane of three CBFM condensed phases (the pure 2e-CP s+ and 2h-CP s- BE condensate phases and a mixed phase ss) along with the normal (ternary BF non-Fermi-liquid) phase n.

superfluid) condensed state, while  $n_0(T)$  and  $m_0(T)$  are the BEC order parameters depicting the macroscopic occupation that arises below  $T_c$  in a BE condensate. This  $\Delta(T)$  is precisely the BCS energy gap if the boson-fermion coupling f is made to correspond to  $\sqrt{2V\hbar\omega_D}$ . Note that the BCS and BE  $T_c$ s are the same. Writing (9) for T=0, and dividing this into (9) gives the much simpler f-independent relation involving order parameters normalized in the interaval [0,1]

$$\Delta(T)/\Delta(0) = \sqrt{n_0(T)/n_0(0)} = \sqrt{m_0(T)/m_0(0)} \xrightarrow[T \to 0]{} 1.$$
 (10)

The first equality, apparently first obtained in Ref. [9], simply relates the two heretofore unrelated "half-bell-shaped" order parameters of the BCS and the BEC theories. The second equality [12, 13] implies that a BCS condensate is precisely a BE condensate of equal numbers of 2e- and 2h-CPs. Since (10) is *independent* of the particular two-fermion dynamics of the problem, it can be expected to hold for either SCs and SFs.

#### 3. BCS-BOSE CROSSOVER THEORY

The crossover theory (defined by two simultaneous equations, the gap and number equations) was introduced by many authors beginning in 1967 with Friedel and

co-authors [41]; for a review see Ref. [42]. The critical temperature  $T_c$  is defined by  $\Delta(T_c) = 0$ , and is to be determined self-consistently with  $\mu(T_c)$ . The two equations to be solved, in 2D for the Cooper/BCS model interaction, are [43]

$$1 = \lambda \int_0^{\frac{\hbar\omega_D}{2k_BT_c}} dx \frac{\tanh x}{x} \quad (\text{if } \mu > \hbar\omega_D); \quad 1 = \lambda \int_{\frac{-\mu(T_c)}{2k_BT_c}}^{\frac{\hbar\omega_D}{2k_BT_c}} dx \frac{\tanh x}{2x}, \quad (\text{if } \mu < \hbar\omega_D)$$

$$\tag{11}$$

$$\int_0^\infty \frac{d\epsilon}{\exp[\epsilon - \mu(T_c)/2k_B T_c] + 1} = 1. \tag{12}$$

The last integral can be done analytically, and leaves

$$\mu(T_c) = k_B T_c \ln(e^{E_F/k_B T_c} - 1). \tag{13}$$

The  $\mu(T_c)$  is then eliminated (numerically) from (11) to give  $T_c$  as a function of  $\lambda$ . Using  $\hbar\omega_D/E_F=0.05$  as a typical value for cuprates, increasing  $\lambda$  makes  $\mu(T_c)$  decrease from its weak-coupling (where  $T_c\to 0$ ) value of  $E_F$  down to  $\hbar\omega_D$  when  $\lambda\simeq 56$ , an unphysically large value. Fig. 2 displays  $T_c$  (in units of  $T_F$ ) as function of  $\lambda$ .

# 4. GAP EQUATION

Curiously, the standard procedure in all SC and SF theories of many-fermions is to ignore 2h-CPs altogether. Indeed, the BCS gap equation for all T can be derived without them. Neglecting in (6) all terms containing  $m_0(T)$ ,  $E_-(0)$  and  $f_-(\epsilon)$  leaves an  $\Omega(T, L^d, \mu, N_0)$  defining an incomplete BFM. Minimizing it over  $N_0$  (for fixed total electron number N) requires that  $\partial\Omega/\partial N_0 = 0$  or  $\partial\Omega/\partial n_0 = 0$ , which becomes

$$\int_0^\infty d\epsilon N(\epsilon) \left[ -1 + \frac{2\exp\{-\beta E(\epsilon)\}}{1 + \exp\{-\beta E(\epsilon)\}} \right] \frac{dE(\epsilon)}{dn_0} + \left[ E_+(0) - 2\mu \right] = 0$$

or

$$2\left[E_{+}(0) - 2\mu\right] = f^{2} \int_{E_{f}}^{E_{f} + \delta\varepsilon} d\epsilon N(\epsilon) \frac{1}{E(\epsilon)} \tanh \frac{1}{2} \beta E(\epsilon). \tag{14}$$

Using (4) yields precisely the BCS gap equation for all T, namely

$$1 = \lambda \int_0^{\hbar\omega_D} d\xi \frac{1}{\sqrt{\xi^2 + \Delta^2(T)}} \tanh \frac{1}{2} \beta \sqrt{\xi^2 + \Delta^2(T)}$$
 (15)

where  $\xi \equiv \epsilon - \mu$ , provided one picks  $E_f = \mu$ , since  $\lambda \equiv f^2 N(0)/2\delta\varepsilon$  while  $\delta\varepsilon = \hbar\omega_D$ . The companion number equation follows from the last equation of (7) and will thus be

$$n = n_f(T) + 2n_B(T) \tag{16}$$

where  $n_f(T)$  is the number density of unpaired electrons

$$n_f(T) \equiv \int_0^\infty d\epsilon N(\epsilon) \left[1 - \frac{\epsilon - \mu}{E(\epsilon)} \tanh \frac{1}{2} \beta E(\epsilon)\right]$$
 (17)

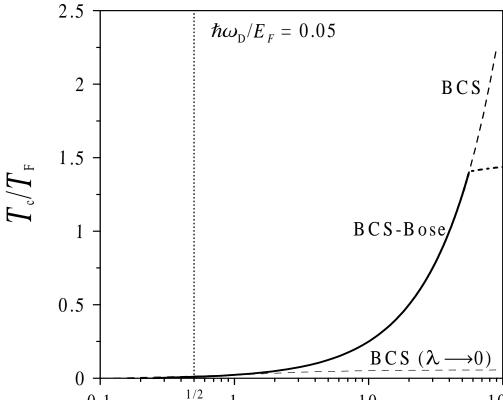


Figure 2. Critical SC temperatures  $T_c$  in units of  $T_F$  for the BCS-Bose crossover theory (full curve), the BCS value from the exact implicit equation (Ref. [21], p. 447)  $1 = \lambda \int_0^{\hbar\omega_D/2k_BT_c} dxx^{-1} \tanh x$  (upper dashed curve) and its weak-coupling solution  $T_c \simeq 1.134\hbar\omega_D \exp(-1/\lambda)$  (lower dashed curve). The dot-dashed "appendage" signals a breakdown in the BCS/Cooper interaction model when  $\mu(T_c)$  turns negative, as the Fermi surface at  $\mu$  then washes out. The value of  $\lambda = 1/2$  marked is the maximum possible value allowed [45] for this interaction model just short of lattice instability.

while the number density of composite bosons, both with K=0 and with K>0, is

$$n_B(T) \equiv n_0(T) + n_{B+}(T); \qquad n_{B+}(T) \equiv \int_{0+}^{\infty} d\varepsilon M(\varepsilon) \frac{1}{e^{\beta [E_+(0) - 2\mu + \varepsilon]} - 1}.$$
 (18)

Note that the number equation  $n = n_f(T) + 2n_B(T)$  differs from (12) of the previous section which follows from  $n = n_f(T)$  only.

Similarly, ignoring 2e-CPs and keeping only 2h-CPs leads to  $\Omega(T, L^d, \mu, M_0)$  which to minimize over  $M_0$  requires that  $\partial\Omega/\partial M_0 = \partial\Omega/\partial m_0 = 0$  and, since  $E(\xi) \equiv E(-\xi)$ . This again leads to (15) but now with the companion number equation

$$m = n_f(T) - 2m_B(T) \tag{19}$$

with the same previous  $n_f(T)$  and where

$$m_B(T) \equiv m_0(T) + m_{B+}(T); \qquad m_{B+}(T) \equiv \int_{0+}^{\infty} d\varepsilon M(\varepsilon) \frac{1}{e^{\beta[2\mu - E_-(0) + \varepsilon]} - 1}.$$
 (20)

However, ignoring either 2e- or 2h-CPs does *not* give the entire BCS ground-state energy, as we now show.

### 5. CONDENSATION ENERGY

The T=0 condensation energy per unit volume according to the CBFM (i.e., with both 2e- and 2h-CPs) is

$$\frac{E_s - E_n}{L^d} = \frac{\Omega_s(T=0) - \Omega_n(T=0)}{L^d}$$
 (21)

since for any T the Helmholtz free energy  $F = \Omega + \mu N = E - TS$ , with S the entropy, and  $\mu$  is the same for either superconducting s or normal n phases with internal energies  $E_s$  and  $E_n$ , respectively. In the normal phase  $n_0 = 0$ ,  $m_0 = 0$  so that  $\Delta(T) = 0$  for all  $T \geq 0$ , and (6) reduces to

$$\frac{\Omega_n(T=0)}{L^d} = \int_0^\infty d\epsilon N(\epsilon) [\epsilon - \mu - |\epsilon - \mu|] = 2 \int_0^\mu d\epsilon N(\epsilon) [\epsilon - \mu] = 2 \int_{-\mu}^0 d\xi N(\xi) \xi. \tag{22}$$

For the superconducting phase at T=0, and when  $n_0(T)=m_0(T)$  and  $n_B(T)=m_B(T)$  hold, one deduces from (4) and (6) that  $\mu=E_f$ . Letting  $\Delta(T=0)\equiv\Delta$  in (6) and putting  $\delta\varepsilon\equiv\hbar\omega_D$  while using (4) gives for the superconducting phase

$$\frac{\Omega_s(T=0)}{L^d} = 2\hbar\omega_D n_0(0) + \int_{-\mu}^{\infty} d\xi N(\xi) \left(\xi - \sqrt{\xi^2 + \Delta^2}\right) 
= 2\hbar\omega_D n_0(0) + 2\int_{-\mu}^{-\hbar\omega_D} d\xi N(\xi)\xi - 2\int_0^{\hbar\omega_D} d\xi N(\xi)\sqrt{\xi^2 + \Delta^2}.$$
(23)

Subtracting (22) from (23) and putting  $N(\xi) \cong N(0)$ , the density of electronic states at the Fermi surface, one is left with

$$\frac{E_s - E_n}{L^d} = 2\hbar\omega_D n_0(0) + 2N(0) \int_0^{\hbar\omega_D} d\xi \left(\xi - \sqrt{\xi^2 + \Delta^2}\right)$$
 (CBFM). (24)

Employing Eq. (2), p. 158 of Ref. [44] the integral becomes

$$\frac{(\hbar\omega_D)^2}{2} - \frac{1}{2}\hbar\omega_D\sqrt{(\hbar\omega_D)^2 + \Delta^2} + \frac{1}{2}\Delta^2\ln\frac{\Delta}{\hbar\omega_D + \sqrt{(\hbar\omega_D)^2 + \Delta^2}}$$

$$\xrightarrow{\Delta\to 0} \frac{1}{2}\Delta^2\ln\left(\frac{\Delta}{2\hbar\omega_D}\right) - \frac{1}{4}\Delta^2 - \frac{1}{16}\frac{\Delta^4}{(\hbar\omega_D)^2} + O\left(\frac{\Delta^6}{[\hbar\omega_D]^4}\right). \tag{25}$$

Using (9) for T=0 and weak coupling  $f\to 0$  implies that  $\Delta=f\sqrt{n_0(0)}=f\sqrt{m_0(0)}\to 0$  so that (24) yields the expansion

$$\frac{E_s - E_n}{L^d} \xrightarrow{\Delta \to 0} 2\hbar\omega_D n_0(0) 
+ 2N(0) \left[ \frac{1}{2} \Delta^2 \ln \left( \frac{\Delta}{2\hbar\omega_D} \right) - \frac{1}{4} \Delta^2 - \frac{1}{16} \frac{\Delta^4}{(\hbar\omega_D)^2} + O\left( \frac{\Delta^6}{[\hbar\omega_D]^4} \right) \right] \quad \text{(CBFM)}. \quad (26)$$

Given that for small  $\lambda$ 

$$\Delta = \frac{\hbar \omega_D}{\sinh(1/\lambda)} \xrightarrow{\lambda \to 0} 2\hbar \omega_D \exp(-1/\lambda)$$
 (27)

the log term in (26) is just

$$\ln\left(\frac{\Delta}{2\hbar\omega_D}\right) = -\frac{2\hbar\omega_D}{f^2N(0)} \tag{28}$$

since

$$\lambda \equiv VN(0) = \frac{f^2N(0)}{2\hbar\omega_D} \tag{29}$$

so that (26) finally simplifies to

$$\frac{E_s - E_n}{L^d} \xrightarrow{\Delta \to 0} -\frac{1}{2}N(0)\Delta^2 \left[ 1 + \frac{1}{4} \left( \frac{\Delta}{\hbar \omega_D} \right)^2 + O\left( \frac{\Delta}{\hbar \omega_D} \right)^4 \right]$$
 (CBFM). (30)

By contrast, the original BCS expression from Eq. (2.42) of Ref. [6] is

$$\frac{E_s - E_n}{L^d} = N(0)(\hbar\omega_D)^2 \left[ 1 - \sqrt{1 + (\Delta/\hbar\omega_D)^2} \right]$$
 (BCS)

which on expansion leaves

$$\frac{E_s - E_n}{L^d} \xrightarrow{\lambda \to 0} -\frac{1}{2}N(0)\Delta^2 \left[ 1 - \frac{1}{4} \left( \frac{\Delta}{\hbar \omega_D} \right)^2 + O\left( \frac{\Delta}{\hbar \omega_D} \right)^4 \right]$$
 (BCS). (32)

Thus, the CBFM condensation energy (30), and consequently its ground-state energy, is lower (or larger in magnitude) than the BCS result (32). Therefore, the CBFM satisfies a prime expectation of any theory that improves upon BCS, which being based on a trial wave function gives a ground-state energy which is a rigorous upper bound to the exact energy associated with the BCS Hamiltonian ground state. Consequently, there is no a priori reason why the CBFM is limited to weak coupling, at least for all  $\lambda < 1/2$  [45].

What happens on ignoring either 2e- or 2h-CPs, as seems to be common practice in theories of SCs and SFs? Starting from (6) for T=0, and following a similar procedure to arrive at (23) but without 2h-CPs such that  $f_-=0$ ,  $m_0(0)=0$  and  $n_0(0)=\Delta^2/f^2$ , one gets

$$\left[\frac{\Omega_s(T=0)}{L^d}\right]_+ = \hbar\omega_D n_0(0) + 2\int_{-\mu}^0 d\xi N(\xi)\xi + N(0)\int_0^{\hbar\omega_D} d\xi \left(\xi - \sqrt{\xi^2 + \Delta^2}\right).$$
(33)

Subtracting (22) from (33) gives

$$\left[\frac{E_s - E_n}{L^d}\right]_+ = \hbar\omega_D n_0(0) + N(0) \int_0^{\hbar\omega_D} d\xi \left(\xi - \sqrt{\xi^2 + \Delta^2}\right)$$
(34)

which is just one half the full CBFM result (24). Furthermore, if  $[(E_s - E_n)/L^d]_-$  is the contribution from 2h-CPs alone, assuming now that  $f_+ = 0$  and  $n_0(0) = 0$  we eventually arrive at precisely rhs of (34) but with  $m_0(0) = \Delta^2/f^2$  in place of  $n_0(0)$ . Hence

$$\left[\frac{E_s - E_n}{L^d}\right]_{+} = \left[\frac{E_s - E_n}{L^d}\right]_{-} \xrightarrow{\lambda \to 0} -\frac{1}{4}N(0)\Delta^2 \left[1 + \frac{1}{4}\left(\frac{\Delta}{\hbar\omega_D}\right)^2 + O\left(\frac{\Delta}{\hbar\omega_D}\right)^4\right] (35)$$

which again is just one half the full CBFM condensation energy (30) that in leading order in  $\Delta$  was found to be the full BCS condensation energy.

Including both 2e- and 2h-CPs gave similarly striking conclusions on generalizing [22, 23] the ordinary [18] CP problem from unrealistic infinite-lifetime pairs to the physically expected finite-lifetime ones.

## 6. CONCLUSIONS

The recent "complete boson-fermion model" (CBFM) contains as a special case the BCS-Bose crossover theory which, at least for the Cooper/BCS model interaction, predicts virtually the same  $T_c$ s to well beyond physically unreasonable values of coupling than the allegedly less general BCS theory where the number equation is replaced by the assumption that  $\mu = E_F$ .

The CBFM reveals that, while the BCS gap equation for all temperatures follows rigorously without either electron or hole pairs, the resulting T=0 condensation energy is only one half the entire BCS value. In view of this, if BEC is at all relevant in SCs and SFs taken as many-fermion systems where pairing into bosons undoubtedly occurs, two-hole CPs cannot and must not be ignored.

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## REFERENCES

- [1] M. de Llano, in *Frontiers in Superconductivity Research* (ed. B.P. Martins) (Nova Science Publishers, NY, 2004). Available in cond-mat/0405071.
- [2] J.M. Blatt, Theory of Superconductivity (Academic, New York, 1964).
- [3] M.R. Schafroth, Phys. Rev. **96**, 1442 (1954).
- $[4]\,$  M.R. Schafroth, et al., Helv. Phys. Acta  ${\bf 30},\,93$  (1957).
- [5] M.R. Schafroth, Sol. State Phys. 10, 293 (1960).

- [6] J. Bardeen, L.N. Cooper & J.R. Schrieffer, Phys. Rev. 108, 1175 (1957).
- [7] N.N. Bogoliubov, JETP **34**, 41 (1958).
- [8] N.N. Bogoliubov, V.V. Tolmachev & D.V. Shirkov, Fortschr. Phys. **6**, 605 (1958); and also in *A New Method in the Theory of Superconductivity* (Consultants Bureau, NY, 1959).
- [9] J. Ranninger & S. Robaszkiewicz, Physica B **135**, 468 (1985).
- [10] R. Friedberg & T.D. Lee, Phys. Rev. B 40, 6745 (1989).
- [11] R. Friedberg, et al., Phys. Lett. A 152, 417 and 423 (1991).
- [12] V.V. Tolmachev, Phys. Lett. A **266**, 400 (2000).
- [13] M. de Llano & V.V. Tolmachev, Physica A **317**, 546 (2003).
- [14] J. Batle, et al., Cond. Matter Theories 18, 111 (2003). cond-mat/0211456.
- [15] M. Casas, et al., Phys. Lett. A **245**, 5 (1998).
- [16] M. Casas, et al., Physica A **295**, 146 (2001).
- [17] M. Casas, et al., Sol. State Comm. 123, 101 (2002).
- [18] L.N. Cooper, Phys. Rev. **104**, 1189 (1956).
- [19] S.K. Adhikari, et al., Phys. Rev. B 62, 8671 (2000).
- [20] S.K. Adhikari, et al., Physica C **351**, 341 (2001).
- [21] A.L. Fetter & J.D. Walecka, Quantum Theory of Many-Particle Systems (McGraw-Hill, New York, 1971).
- [22] M. Fortes, et al., Physica C **364-365**, 95 (2001).
- [23] V.C. Aguilera-Navarro, et al., Sol. St. Comm. 129, 577 (2004).
- [24] N.N. Bogoliubov, N. Cim. 7, 794 (1958).
- [25] D. Vollkardt & P. Wölfle, *The Superfluid Phases of Helium 3* (Taylor & Francis, London, 1990).
- [26] E.R. Dobbs, Helium Three (Oxford University Press, Oxford, UK, 2000).
- [27] M.J. Holland, B. DeMarco & D.S. Jin, Phys. Rev. A 61, 053610 (2000).
- [28] K.M. O'Hara, S.L. Hammer, M.E. Ghem, S.R. Granade & J.E. Thomas, Science **298**, 2179 (2002).
- [29] K.E. Strecker, G.B. Partridge & R.G. Hulet, Phys. Rev. Lett. **91**, 080406 (2003).
- [30] M. Holland, S.J.J.M.F. Kokkelmans, M.L. Chiofalo & R. Walser, Phys. Rev. Lett. 87, 120406 (2001).
- [31] E. Timmermans, K. Furuya, P.W. Milonni & A.K. Kerman, Phys. Lett. A 285, 228 (2001).
- [32] M.L. Chiofalo, S.J.J.M.F. Kokkelmans, J.N. Milstein & M.J. Holland, Phys. Rev. Lett. 88, 090402 (2002).
- [33] Y. Ohashi & A. Griffin, Phys. Rev. Lett. 89, 130402 (2002).
- [34] L. Pitaevskii & S. Stringari, Science 298, 2144 (2002).
- [35] M. Greiner, C.A. Regal & D.S. Jin, Nature 426, 537 (2003).
- [36] C.A. Regal, M. Greiner & D.S. Jin, Phys. Rev. Lett. **92**, 040403 (2004).
- [37] M.W. Zwierlein, C. A. Stan, C. H. Schunck, S.M. F. Raupach, S. Gupta, Z.

- Hadzibabic & W. Ketterle, Phys. Rev. Lett. **91**, 250401 (2003).
- [38] S. Jochim, M. Bartenstein, A. Altmeyer, G. Hendl, S. Riedl, C. Chin, J. Hecker Denschlag & R. Grimm, Science 302, 2101 (2003).
- [39] N.N. Bogoliubov, J. Phys. (USSR) 11, 23 (1947).
- [40] M. Casas, M. de Llano & V.V. Tolmachev, to be published.
- [41] J. Labbé, S. Barisic & J. Friedel, Phys. Rev. Lett. 19, 1039 (1967).
- [42] M. Randeria, in *Bose-Einstein Condensation*, ed. A. Griffin *et al.* (Cambridge University, Cambridge, 1995) p. 355.
- [43] F.J. Sevilla, PhD Thesis (UNAM, 2004) unpublished.
- [44] A. Jeffrey, *Handbook of Mathematical Formulas and Integrals* (Academic Press, Newcastle, UK, 1995).
- [45] A.B. Migdal, JETP 7, 996 (1958).